Subject: Re: Similarity heatmap

Posted by thomas on Wed, 02 Dec 2020 19:33:17 GMT

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Currently, DataWarrior cannot show heatmaps also it is able to perform a hierarchical clustering. Probably, heatmaps will come some time in the future. Protein similarity is another thing that is not likely to be added soon, because DataWarrior focuses on small molecules. Proteins will play a role soon, but as target for docking only.